ODEs and decompositions

Learning outcomes:

- Look at decompositions of matrix eqautions and how they can be used to solve linear equations.

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LU decomposition

Again we want to solve $\textbf{Ax - b} = 0$

Suppose we can rewrite this as

$$\begin{pmatrix} u_{00} & u_{01} & u_{02} \\ 0 & u_{11} & u_{12} \\ 0 & 0 & u_{22} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix} - \begin{pmatrix} d_0 \\ d_1 \\ d_2 \end{pmatrix} = 0$$

which looks similar to Gauss elmination.

In matrix notation

$$\textbf{Ux - d} = \mathbf{0}$$

.

Now, assume there is a lower diagonal matrix $\textbf{L}$ with '1's on the diagonal

$$\begin{pmatrix} 1 & 0 & 0 \\ l_{10} & 1 & 0 \\ l_{20} & l_{21} & 1 \end{pmatrix}$$

that has the property that, premultiplying by $\textbf{L}$ we get

$$\mathbf{LUx} - \mathbf{Ld} = \mathbf{Ax} - \mathbf{b}$$

LU decomposition

To ensure that

$$\mathbf{LUx} - \mathbf{Ld} = \mathbf{Ax} - \mathbf{b}$$

we require that

$$\mathbf{LU} = \mathbf{A}$$

and

$$\mathbf{Ld} = \mathbf{b}$$

Triangularization by Gauss elimination

When we do the Gauss elimination method, we actually find all the elements of $\textbf{L}$, we just need to store them.
It is the inverse of the matrix we would need to multiply $\textbf{b}$ by to get the correct RHS in the Gauss elmination method.

Let us take an initial augmented matrix, and record the values that we would scale the $\textbf{b}$ matrix by if it were there:

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix}$$

pivoting around row 0, we remove all entries below the diagonal entry in column 0, doing this we scaled the $\textbf{b}$ matrix by the ratios shown on the right

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & a'_{21} & a'_{22} & a'_{23} \\ 0 & a'_{31} & a'_{32} & a'_{33} \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{10}}{a_{00}} & & & \\ \frac{a_{20}}{a_{00}} & & & \\ \frac{a_{30}}{a_{00}} & & & \end{pmatrix}$$

Matrix after pivoting around row 0

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & a'_{21} & a'_{22} & a'_{23} \\ 0 & a'_{31} & a'_{32} & a'_{33} \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{10}}{a_{00}} & & & \\ \frac{a_{20}}{a_{00}} & & & \\ \frac{a_{30}}{a_{00}} & & & \end{pmatrix}$$

Then pivoting around row 1 we remove elements below the diagonal in column 1, and subtract multiples of the 2nd row of $\textbf{b}$ as shown in the right hand matrix

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & a''_{32} & a''_{33} \end{pmatrix} \qquad \begin{pmatrix} 1 & & & \\ \frac{a_{10}}{a_{00}} & 1 & & \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{10}} & & \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{10}} & & \end{pmatrix}$$

pivoting around row 2

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & 0 & a'''_{33} \end{pmatrix} \qquad \begin{pmatrix} 1 & & & \\ \frac{a_{10}}{a_{00}} & 1 & & \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{11}} & 1 & \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{11}} & \frac{a''_{32}}{a''_{22}} & \end{pmatrix}$$

we had got to

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & 0 & a'''_{33} \end{pmatrix} \qquad \begin{pmatrix} 1 & & & \\ \frac{a_{10}}{a_{00}} & 1 & & \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{11}} & 1 & \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{11}} & \frac{a''_{32}}{a''_{22}} & \end{pmatrix}$$

if we fill in the rest of the matrix on the right we have

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & 0 & a'''_{33} \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{10}}{a_{00}} & 1 & 0 & 0 \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{11}} & 1 & 0 \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{11}} & \frac{a''_{32}}{a''_{22}} & 1 \end{pmatrix}$$

We can show for a real system that this new matrix is $\textbf{L}$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{10}}{a_{00}} & 1 & 0 & 0 \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{11}} & 1 & 0 \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{11}} & \frac{a''_{32}}{a''_{22}} & 1 \end{pmatrix} \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & 0 & a'''_{33} \end{pmatrix} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$\mathbf{LU} = \mathbf{A}$$

and

$$\mathbf{Ld} = \mathbf{b}$$

- So only very minor changes in the Gauss elimination code are needed.
- You can store the nondiagonal elements of $\textbf{L}$ in what would be the zero elements of the row echelon matrix.

LU decomposition

An advantage of LU decompostion is we calculate $\textbf{L}$ and $\textbf{U}$ once, then we can easily find $\textbf{x}$ for any $\textbf{b}$

Having $\textbf{L}$ we can solve $\textbf{Ld} = \textbf{b}$ for $\textbf{d}$ by forward substitution

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{10}}{a_{00}} & 1 & 0 & 0 \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{11}} & 1 & 0 \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{11}} & \frac{a''_{32}}{a''_{22}} & 1 \end{pmatrix} \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

i.e. multiplying out the equations starting from the top row.

Then, having constructed $\textbf{d}$ for the given $\textbf{b}$ we continue exactly like in Gauss Elimination using back substitution to find $\textbf{x}$

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & 0 & a'''_{33} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \end{pmatrix}$$

We can directly use this method in the Eigen library.

```
#include
#include
using namespace std;
using namespace Eigen;
int main()
{
    Matrix3f A;
    Vector3f b;
    A << 1,2,3,  4,5,6,  7,8,10;
    b << 3, 3, 4;
    cout << "Here is the matrix A:\n" << A << endl;
    cout << "Here is the vector b:\n" << b << endl;
    Vector3f x = A.fullPivLu().solve(b);
    cout << "The solution is:\n" << x << endl;
}
```

The reference for the full LU decompositon method is here (https://eigen.tuxfamily.org/dox/classEigen_1_1FullPivLU.html).

LU decomposition

We can use LU decomposition to find the inverse of a matrix, by setting b to the columns of the identity matrix, I.

For example we get the first column of $\textbf{A}^{-1}$ by using $\textbf{b}^T = (1,0,0,0)$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{a_{10}}{a_{00}} & 1 & 0 & 0 \\ \frac{a_{20}}{a_{00}} & \frac{a'_{21}}{a'_{11}} & 1 & 0 \\ \frac{a_{30}}{a_{00}} & \frac{a'_{31}}{a'_{11}} & \frac{a''_{32}}{a''_{22}} & 1 \end{pmatrix} \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

i.e. multiplying out the equations starting from the top row.

Then, having constructed $\textbf{d}$ for the given $\textbf{b}$ we continue exactly like in Gauss Elimination using back substitution to find $\textbf{x}$

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ 0 & a'_{11} & a'_{12} & a'_{13} \\ 0 & 0 & a''_{22} & a''_{23} \\ 0 & 0 & 0 & a'''_{33} \end{pmatrix} \begin{pmatrix} A^{-1}_{00} \\ A^{-1}_{10} \\ A^{-1}_{20} \\ A^{-1}_{30} \end{pmatrix} = \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \end{pmatrix}$$

Then we build the other columns of $\textbf{A}^{-1}$ from the other unit vectors.

If you want to understand the LU decomposition clearly, adapt a gauss-elim type code to also perform LU decomposition

Find the inverse of this matrix using LU decomposition

$$\begin{pmatrix} 2 & 2 & 4 & -2 \\ 1 & 3 & 2 & 4 \\ 3 & 1 & 3 & 1 \\ 1 & 3 & 4 & 2 \end{pmatrix}$$

Check your solution is correct by comparison to Gauss-Jordan or Eigen / numpy libraries. Note you can also get the determinant from LU decomposition - how?

QR decomposition

Why another decomposition???

This decomposition is part of the 'QR' algorithm to find the eigenvalues and vectors of a matrix.

Any real square matrix A may be decomposed as

$$\mathbf{A} = \mathbf{QR},$$

where

- $\textbf{Q}$ is an orthogonal matrix (its columns are orthogonal unit vectors meaning $\textbf{Q}^t\textbf{Q} = I$)
- $\textbf{R}$ is an upper triangular matrix (also called right triangular matrix).

If $\textbf{A}$ is invertible, then the factorization is unique if we require the diagonal elements of $\textbf{R}$ to be positive.

QR decomposition

Gram–Schmidt orthogonalisation.

You may remember this from linear algebra - we build an orthogonal basis by sucessively projecting out previous basis vectors

We can scan across the columns of our matrix $\textbf{A}$ and remove the components of any previous column by subtracting the dot product.

Take an initial matrix $\textbf{A}$

$$\mathbf{A} = \begin{pmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{pmatrix}$$

First we'll make an orthogonal matrix $\textbf{U}$, we'll keep the first column.

$$\mathbf{U} = \begin{pmatrix} 12 & ? & ? \\ 6 & ? & ? \\ -4 & ? & ? \end{pmatrix}$$

To get the 2nd column orthogonal, we subtract the projection of the second column onto the first column from the 2nd column.

To get the 2nd column orthogonal, we subtract the projection of the second column onto the first column from the 2nd column.

$$\mathbf{U} = \begin{pmatrix} 12 & -51 - \mathrm{proj}_{col_1} & ? \\ 6 & 167 - \mathrm{proj}_{col_1} & ? \\ -4 & 24 - \mathrm{proj}_{col_1} & ? \end{pmatrix}$$

where the projection onto the first column is given by

$$\begin{aligned} proj_{col_1} &= \left\langle \mathbf{col}_2 \cdot \frac{\mathbf{col}_1}{||col_1||} \right\rangle \frac{\mathbf{col\_1}}{||col_1||} \\ &= \left\langle (-51, 167, 24) \cdot \begin{pmatrix} 12 \\ 6 \\ 4 \end{pmatrix} \right\rangle (12, 6, 4) \frac{1}{(12^2+6^2+4^2)} \\ &= \frac{294}{196}(12, 6, 4) = (18, 9, -6) \end{aligned}$$

so

$$\mathbf{U} = \begin{pmatrix} 12 & -51 - 18 & ? \\ 6 & 167 - 9 & ? \\ -4 & 24 - -6 & ? \end{pmatrix} = \begin{pmatrix} 12 & -69 & ? \\ 6 & 158 & ? \\ -4 & 30 & ? \end{pmatrix}$$

Two get the 3rd column orthogonal, we subtract the projection of the third column onto the first two columns.

$$\mathbf{U} = \begin{pmatrix} 12 & -69 & 4 - (\text{proj}_{col_1} + \text{proj}_{col_2}) \\ 6 & 158 & -68 - (\text{proj}_{col_1} + \text{proj}_{col_2}) \\ -4 & 30 & -41 - (\text{proj}_{col_1} + \text{proj}_{col_2}) \end{pmatrix}$$
$$= \begin{pmatrix} 12 & -69 & -58/5 \\ 6 & 158 & 6/5 \\ -4 & 30 & -33 \end{pmatrix}$$

Now we make each column a unit vector to get the orthogonal matrix $\textbf{Q}$

$$\mathbf{Q} = \begin{pmatrix} \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} & \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} & \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \end{pmatrix} = \begin{pmatrix} 6/7 & -69/175 & -58/175 \\ 3/7 & 158/175 & 6/175 \\ -2/7 & 6/35 & -33/35 \end{pmatrix}.$$

Remember, we wanted

$$\mathbf{A} = \mathbf{Q}\mathbf{R},$$

if we premultiply by $\textbf{Q}^T$ we get

$$\mathbf{Q}^T\mathbf{A} = \mathbf{Q}^T\mathbf{Q}\mathbf{R},$$

but for an orthogonal matrix $\textbf{Q}^T\textbf{Q} = \textbf{I}$ so we have

$$\mathbf{Q}^T\mathbf{A} = \mathbf{R},$$

and we can find $\textbf{R}$ my mulitplying our original matrix $\textbf{A}$ and the (transposed) orthogonal matrix we just found.

$$R = Q^T A = \begin{pmatrix} 14 & 21 & -14 \\ 0 & 175 & -70 \\ 0 & 0 & 35 \end{pmatrix}.$$

QR usage and exercise

Real life examples normally use [Householder transformations (https://en.wikipedia.org/wiki/Householder_transformation)](https://en.wikipedia.org/wiki/Householder_transformation) rather than Gramm-Schmidt orthogonalisation as they are more numerically stable.

The QR factorization can be used for general least squares curve fitting, as a way of improving the stability of systems of linear equations and as part of an alogrithm to find the eigenvalues and vectors of a matrix.

See if you can write a code to carry out the QR factorization of the matrix that we inverted earlier using Gramm-Schmidt orthogonalisation.

Find the QR decomposition of this matrix:

$$\begin{pmatrix} 2 & 2 & 4 & -2 \\ 1 & 3 & 2 & 4 \\ 3 & 1 & 3 & 1 \\ 1 & 3 & 4 & 2 \end{pmatrix}$$

Summary and Further Reading

You should be reading additional material to provide a solid background to what we do in class

All the textbooks contain sections on solving linear equations, for instance chapter 2 of Numerical Recipes (http://apps.nrbook.com/c/index.html).

Note to access numerical recipes you need to have Flash activated - this is ***not*** secure. I'd suggest at a minumum doing this in a separate incognito browser window without any other tabs open.